

One-particle spectral function of electrons in a hot and dense plasma

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A self-consistent determination of the spectral function and the self-energy of electrons in a hot and dense plasma is reported. The self-energy is determined within the approximation of the screened potential. It is shown, that the quasi-particle concept is not an adequate concept for hot and dense plasmas, since the width of the spectral function has to be considered. As an example, the solar core plasma is discussed. An effective quasi-particle picture is introduced and results for the solar core plasma as well as for ICF plasmas are presented.

I. INTRODUCTION

Dense plasmas are intensively studied both in experimental as well as theoretical physics. Typical plasmas of this kind can be found in astrophysical objects like the interior of the sun and the giant planets. On earth, very dense and hot plasmas are investigated in the context of inertial confinement fusion. Furthermore, the electron gas in some metals and semiconductors represents a dense and cold plasma. From the study of dense plasmas, important information about microscopic mechanisms like the interplay between collective effects and collisions can be gained. The consistent description of this interplay is a very challenging task.

In a dense plasma, the propagation of a single-particle excitation is a collective phenomenon which is characterized by the single-particle spectral function. The spectral function for the specie a is given as the discontinuity of the single-particle Green's function at real frequencies

$$A_a(p, \omega) = i\hbar (G_a(p, \omega + i0) - G_a(p, \omega - i0)) \quad . \quad (1)$$

In contrast to the quasi-particle picture, where the spectral function is assumed to be proportional to the δ -function,

$$A_a(p, \omega) = 2\pi \delta(\hbar\omega - E_a(p)) \quad , \quad (2)$$

in dense plasmas the broadening of the spectral function is of great importance, since it describes the finite life time of the excitations in the plasma. Here $E_a(p)$ denotes the quasi-particle energy defined below. The spectral function has a number of interesting properties, which are connected to the thermodynamical properties of the plasma. First of all, there is a frequency sum rule

$$\int_{-\infty}^{\infty} d\omega A_a(p, \omega) = 2\pi \quad . \quad (3)$$

As a consequence, the spectral function gives the probability to find a certain frequency at a given momentum p . Furthermore, the density of states is related to the spectral function by

$$D_a(\omega) = \int \frac{d^3p}{(2\pi)^3} A_a(p, \omega) \quad , \quad (4)$$

leading to the so called density relation

$$n_a(\mu_a, \beta) = \int_{-\infty}^{\infty} \frac{d\hbar\omega}{2\pi} f_a(\omega) D_a(\omega) \quad , \quad (5)$$

where f_a denotes the Fermi distribution function. For a system with a given density n_a , this relation can be used to fix the corresponding chemical potential μ_a . Additional thermodynamic properties can be derived, e.g. the equation of state can be found. Therefore, the equation of state can be improved taking into account many-particle effects via an appropriate spectral function.

The spectral function for dense systems has been determined in the context of nuclear physics as well as solid state physics. In nuclear physics [1], the spectral function of nuclear matter has been studied extensively. It has been shown that the spectral function exhibits a complex energy dependence, which cannot be incorporated in a simple quasi-particle

picture. Effects of higher order correlations like the pairing instability on the spectral function have been found. The influence of these pairing effects are reduced if the broadening of the spectral function increases.

In solid state physics, extensive studies of the spectral function have been carried out within the Hubbard-model [2] and the t-J model [3]. Thermally broadened quasi-particles have been found at high temperatures. Zimmermann et al. [4] performed an expansion with respect to the width of the spectral function to get a so called extended quasi-particle picture, but its use is limited to small deviations from the quasi-particle regime. A calculation similar to the one reported here, has been carried out by Barth and Holm [5]. They applied their calculation to the electron gas at zero temperature. In solid state physics the spectral function can be measured using angle-resolved photoemission spectroscopy.

II. SPECTRAL FUNCTION AND SELF-ENERGY

The single-particle Green's function of the specie a reads

$$G_a(p, z) = \left(\hbar z - \frac{\hbar^2 p^2}{2m_a} - \Sigma_a(p, z) \right)^{-1}. \quad (6)$$

The medium modifications enter via the self-energy Σ_a ,

$$\int d\bar{1} \Sigma_a(1\bar{1}) G_a(\bar{1}1') = - \sum_b \int d2 V(1-2) G_{ab}(121'2^+) \quad (7)$$

where higher order correlations are hidden in the two particle Green's function G_{ab} . The numbers label the position and time variables and the potential V denotes the Coulomb-Potential. The spectral function can be related to the self-energy $\Sigma_a(p, \omega)$ via Dyson's equation

$$A_a(p, \omega) = \frac{2 \operatorname{Im} \Sigma_a(p, \omega)}{\left(\hbar \omega - \frac{\hbar^2 p^2}{2m_a} - \operatorname{Re} \Sigma_a(p, \omega) \right)^2 + (\operatorname{Im} \Sigma_a(p, \omega))^2}. \quad (8)$$

This relation shows, that the imaginary part of the self-energy plays the role of a width of the spectral function while the real part acts as the shift of the free dispersion relation. Different approximations for the self-energy apply for different systems taking into account different collective mechanisms. For high density systems interacting via the Coulomb potential, Hedin [6] proposed the so called GW approximation where polarization effects are considered. In nuclear matter, particle-particle correlations are the leading mechanisms as was pointed out by Galitski [7]. Therefore, a T-matrix approximation of the self-energy has to be used. A consistent determination of the spectral function using this approximation for the self-energy was performed by Alm et al. [1].

Within the GW approximation, the correlated part of the self-energy is determined by

$$\Sigma_a^{corr}(p, z) = - \int_{-\infty}^{\infty} \frac{d\omega' d\omega}{(2\pi)^2} \int \frac{d^3 q}{(2\pi)^3} V(q) \frac{2 \operatorname{Im} \epsilon^{-1}(q, \omega') A_a(\vec{p} - \vec{q}, \omega) (1 + n_B(\omega') - f_a(\omega))}{z - \omega' - \omega}, \quad (9)$$

whereas the corresponding quasi-particle expression is given by

$$\Sigma_a^{corr, QT}(p, z) = - \int_{-\infty}^{\infty} \frac{d\omega'}{(2\pi)} \int \frac{d^3 q}{(2\pi)^3} V(q) \frac{2 \operatorname{Im} \epsilon^{-1}(q, \omega') (1 + n_B(\omega') - f_a(E_a(\vec{p} - \vec{q})))}{z - \omega' - E_a(\vec{p} - \vec{q})}, \quad (10)$$

Here, $V(q)$ denotes the Coulomb potential, $n_B(\omega') = (\exp(\beta \omega') - 1)^{-1}$ and f_a the Fermi function of the specie a . The solutions of

$$E_a(p) = \frac{\hbar^2 p^2}{2m_a} + \operatorname{Re} \Sigma_a(p, E_a(p)) \quad (11)$$

defines the quasi-particle energy. Besides the spectral function A_a , medium modifications enter via the dielectric function $\epsilon(q, \omega)$. The set of equations (8) and (9) are to be solved self-consistently. Furthermore, the dielectric function depends on the spectral function as well. Here, the RPA expression for the dielectric function is used, i.e. self-energy effects as well as vertex correction in the polarization function are ignored. The consistency of this approximation

will be discussed below. In the classical limit the dielectric response function can be calculated analytically, yielding [8]:

$$\epsilon(q, \omega) = 1 + \sum_{c=1}^3 \frac{\kappa_c^2}{q^2} \left[1 - 2x_c \exp(-x_c^2) \int_0^{x_c} dt \exp(t^2) + i\sqrt{\pi} x_c \exp(-x_c^2) \right] \quad (12)$$

with the abbreviations $\kappa_c = \sqrt{\frac{Z_c^2 e^2 n_c}{\epsilon_0 k_B T}}$ and $x_c = \frac{\omega}{q} \sqrt{\frac{m_c}{2k_B T}}$. Additional sum rules hold (see [5])

$$\int_{-\infty}^{\infty} d\omega \omega A_a(p, \omega) = E^{HF}(p) \quad , \quad (13)$$

$$\int_{-\infty}^{\infty} d\omega \omega^2 A_a(p, \omega) = \int_{-\infty}^{\infty} d\omega \text{Im} \Sigma_a(p, \omega) + (E^{HF}(p))^2 \quad , \quad (14)$$

which present a convenient check of the numerics involved in the self-consistent solution. $E^{HF}(p) = \hbar^2 p^2 / (2m) + \Sigma^{HF}(p)$ is the quasi-particle energy in Hartree-Fock approximation.

III. SELF-CONSISTENT DETERMINATION OF THE SPECTRAL FUNCTION WITHIN THE GW APPROXIMATION

A. Results for the spectral function

Using the RPA expression as an input, the spectral function can be determined by solving the set of equations (8) and (9) iteratively until stability is reached. To start the iteration, one can use a quasi-particle picture or a lorentzian approximation of the spectral function with a certain width. This width can be used to accelerate the convergence of the iteration method. The self-consistently determined spectral function is given in figure 1 for the solar core plasma. In accordance with solar models [9], the temperature is assumed to be $T_{\odot} = 15.6 \times 10^6$ K and the density $n = 156 \text{ g/cm}^3$. The plasma consists of three components, electrons, protons and alpha-particles, with a hydrogen mass fraction of 33%. The spectral function is shown as a function of the frequency for a fixed momentum. The spectral function is fairly broad, its width is about a fifth of the thermal energy. Since the function is asymmetric, the definition of a width and a shift is to a certain extent ambiguous. The definition of an effective quasi-particle description will be proposed in section IIIB. An undamped quasi-particle is by no means an adequate description of the spectral function. Therefore, the calculation of thermodynamical properties should be based on the spectral function calculated here, instead of a quasi-particle approach. In figure 2, a contour plot of the spectral function as a function of the energy and the momentum is shown. The plot shows that the situation discussed above applies also to higher momenta. It has been found that the above given sum rules are fulfilled within the numerical accuracy.

In figure 3, the self-consistently determined energy is shown as a function of the frequency along with the quasi-particle self-energy. As found earlier [10,11] the quasi-particle self-energy shows a logarithmic singularity at the plasmon energy. Due to the additional integration in the definition of the self-energy the self-consistent one does not exhibit a singularity anymore. This corresponds to results reported by Alm et al. [1], where the spectral function and the self-energy are calculated self-consistently for nuclear matter. Since the forces in nuclear matter are short-ranged, the important feature discussed there is the formation of bound states. This issue is of lower relevance for the high temperatures considered here.

B. Effective quasi-particle picture

For the sake of comparison, we define an effective quasi-particle by fitting the self-consistently determined spectral function to a lorentzian shape. This can be achieved by solving the dispersion relation

$$\omega - \frac{\hbar^2 p^2}{2m_e} - \Sigma_e^F(p) = \Sigma_e^{\text{corr}}(p, \omega) \quad . \quad (15)$$

Here, Σ_e^F denotes the Fock shift. The solution ω_0 of this equation can be regarded as the quasi-particle energy. $\Delta(p)^{\text{eff}} = \text{Re} \Sigma(p, \omega_0)$ and $\Gamma^{\text{eff}}(p) = \text{Im} \Sigma(p, \omega_0)$ are interpreted as the shift and the width of a finite lifetime quasi-particle. However, a lorentzian fit is only a crude approximation to the self-consistent spectral function, e.g. the

thermal average of the effective quasi-particle shift is not exactly the Debye shift $\kappa e^2/2$ contrary to the quasi-particle result [8]. A comparison of the effective quasi-particle shift and the quasi-particle self-energy based on a free dispersion is given in figure 4. Note, that the steep decrease of the quasi-particle self-energy at small momenta is not found in the effective shift, while the high momentum behaviour is almost identical. Therefore, the shift is overestimated in a simple quasi-particle picture using a free dispersion relation. Solving the self-consistency relation of the quasi-particle picture (11), a shift corresponding to the one reported here was found by Fehr et al. [11].

Using the effective shift and width defined above, the temperature and density dependence of the spectral function can be studied. The results are shown in figure 5. The width is given as a function of the density for different temperatures. At small as well as at high densities, the width decreases, showing a restoration of the quasi-particle picture. The maximum in between is shifted to higher densities with increasing temperature. Furthermore, comparing different temperatures at a fixed density, a strong temperature dependence is observed. This implies, that thermal collisions are the driving mechanism behind the broadening of the spectral function.

C. Implications for thermodynamical properties

In a first step, the implications for the electron chemical potential due to the improved determination of the spectral function will be examined. This has important consequences for the so called Salpeter correction [13] to thermonuclear reaction rates. Using the self-consistent spectral function the chemical potential for the solar core plasma is determined from equation (5) to be -146.5 Ryd, whereas the chemical potential of an ideal electron gas would be -142.9 Ryd. Using a quasi-particle approximation it is -146.3 Ryd, showing that the broadening of the spectral function has little influence on the chemical potential. Using the Salpeter correction, i.e considering a Debye-shift only, the chemical potential results in -146.2 Ryd. Therefore, on the level of single particle corrections, the reaction rates can be excellently described by the Salpeter expression. Nevertheless, the dynamics also enter in two-particle corrections, which will be considered in a forthcoming paper [17]. Besides the chemical potential, the effects on the equation of state can be studied.

IV. CONCLUSIONS

The self-consistent determination of the spectral function within the screened potential approximation is reported. For the solar core plasma, the self-consistent spectral function is found to be fairly broad. The quasi-particle picture is not an adequate description of the solar core plasma. Therefore, the calculation of thermodynamic properties of the solar core plasma should be based on the spectral function given above. A lorentzian approximation of the spectral function is defined introducing an effective shift and width. This can be interpreted as a damped quasi-particle description. It has been found, that a quasi-particle description overestimates the self-energy at small momenta to a large extend. Furthermore, the self-consistently determined energy does not exhibit a logarithmic singularity at the plasmon energy contrary to the quasi-particle one.

It has been pointed out, that the scheme given above is not completely self-consistent, since the Green's function in the RPA bubble is not iterated. However, a complete iteration [16] shows that the dielectric function does not obey exactly known properties like sum rules. This is due to the fact, that besides self-energy corrections also vertex corrections are to be included. Within the Green's function method, Baym and Kadanoff [15] developed a technique to construct the vertex correction in a way to fulfill the Ward identities. In this approach the sum rules are automatically obeyed. Unfortunately, the integral equation connected with the vertex corrections is very involved. An alternative approach, starting from the Zubarev formalism of the non-equilibrium statistical operator has been developed, where correlations and collisions are incorporated on the same footing [14]. A compensation of self-energy and vertex corrections to a large extend has been found, justifying the use of the original RPA expression.

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Figure Captions:

Fig.1 Self-consistently determined spectral function of the electrons in the solar core plasma. The momentum p is fixed to $p = 0.21 \frac{1}{a_B}$. The self-consistent result as well as the first iteration step starting from a Lorentzian initialisation of the spectral function are shown.

Fig.2 Contour plot of the self-consistently determined spectral function of the electrons in the solar core plasma. The spectral function is given as a function of frequency and momentum. Note that the spectral function remains fairly broad at higher momenta.

Fig.3 The quasi-particle self-energy and the self-consistently determined self-energy as a function of the frequency at a fixed momentum. Note the logarithmic singularity of the imaginary part of the self-energy at the plasma frequency $\omega_{pl} = \pm 21.15 \text{ Ryd}$.

Fig.4 The effective quasi-particle shift as a function of the wave number in comparison with the quasi-particle shift using a free dispersion relation.

Fig.5 The effective width of the spectral function as a function of the density in the long wavelength limit. The temperature is used as a parameter.





